1-(1-hydroxynaphthalen-2-yl)pentan-1-one

67013-64-3 | DTXSID00284025

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 69.8 °C

Global applicability domain: Inside

Local applicability domain index: 5.95e-01

Confidence level: 6.14e-01

Nearest Neighbors from the Training Set

Image not found
Ethanone, 1-(1-hydroxy-2-naphthalenyl)-
Measured: 101
Predicted: 84.8

Image not found
2-Hydroxybenzophenone
Measured: 40.0
Predicted: 63.7

Image not found
2-Propen-1-one, 1-(2-hydroxyphenyl)-3-phenyl-
Measured: 90.0
Predicted: 77.6

Image not found
Clorophene
Measured: 48.5
Predicted: 52.9